(92)

TEACHING SCHEME AND COURSE CONTENTS

FOR

MASTER OF SCIENCE

IN

CHEMISTRY

DEPARTMENT OF CHEMISTRY

NATIONAL INSTITUTE OF TECHNOLOGY HAMIRPUR (H.P.)

Information of the Course to be introduced

Name of the Department: Chemistry

Details of the Course

The Department of Chemistry intends to start a M.Sc. programme in Chemistry with the aim of providing state of art knowledge in the area of chemical sciences to the students. The programme will provide excellent teaching by the qualified and experienced faculty of this department by touching all the relevant aspects of the chemical sciences. Since the inception of this institute, the department has been actively engaged in research activities and has vast experience of guiding Ph.D scholars in addition to execution of R&D Projects from various funding agencies such as CSIR, UGC,DST and MHRD etc. They have volume of research publications at National and International levels to their credit including books.

Available facilities:

The department has well equipped lab facilities to run PG programme as one programme in chemical technology is already running in the department. Most of the major equipments are available in the department/institute to cater to the practical needs of the course. The duration of the course is of two years which will spans over 4 semesters.

Programme Objective:

- To provide a comprehensive, multi-dimensional post-graduate programme in Chemistry with the aim of producing highly competent professionals with a sound knowledge on the importance of chemistry in technological world.
- To provide hand-on exposure on advanced instrumentation techniques, cutting edge R&D area and promote them for carrying out interdisciplinary works to address national/regional societal issues.
- To inculcate good communication skills, technical/scientific curiosity and knowledge among students via regular presentations, seminars, quizzes, and project discussions.
- To emphasize the importance of studying fundamental science and to promote innovative solutions to the science and technological challenges.

Course Offered

Programme	**M.Sc. in Chemistry**
Year of starting	**July, 2017**
Duration(Total)	**2 years(4 Semesters)**
Admission	**Centralized Counselling through CCMN(Centralized Counselling for M.Sc. admissions to NITs and CFTIs) on the basis of JAM(Joint Admission Test for M.Sc.) Score Or Institute Entrance Test**
Eligibility	• **Bachelor Degree along with Chemistry as one of the subject for at least two years/four semesters** • **At least CGPI of 6.5 on a 10-point scale (or equivalent) or 60% aggregate marks for General/OBC Category Candidates and at least CGPI of 6.0 on a 10-point scale (or equivalent) or 55% aggregate marks for SC/ST and PwD category candidates**
Proposed Intake	**15+5***
Reservation	**As per MHRD norms**

***Sponsored Candidates**

M. Sc. PROGRAMME IN CHEMISTRY
DEPARTMENT OF CHEMISTRY

SEMESTER-I

Course No.	Subject	Teaching Schedule			Hours/Week	Credits
		L	T	P		
CH-500	Inorganic Chemistry-I	3	0	0	3	3
CH-501	Organic Chemistry-I	3	0	0	3	3
CH-502	Physical Chemistry-I	3	0	0	3	3
CH-503	Molecular Spectroscopy	3	0	0	3	3
CH-EL1	Departmental Elective-I	3	0	0	3	3
CH-504	Chemistry Lab-I	0	0	9	9	4
Total		**15**	**0**	**9**	**24**	**19**

SEMESTER-II

Course No.	Subject	Teaching Schedule			Hours/Week	Credits
		L	T	P		
CH-505	Inorganic Chemistry-II	3	0	0	3	3
CH-506	Organic Chemistry-II	3	0	0	3	3
CH-507	Physical Chemistry-II	3	0	0	3	3
CH-EL2	Departmental Elective – II ***(From Department of Chemical Engineering)***	3	0	0	3	3
CH-508	Chemistry Lab-II	0	0	9	9	4
Total		**12**	**0**	**9**	**21**	**16**

SEMESTER-III

Course No.	Subject	Teaching Schedule			Hours/Week	Credits
		L	T	P		
CH-509	Organometallics	3	0	0	3	3
CH-510	Interpretative Molecular Spectroscopy	3	0	0	3	3
CH-511	Molecular Energetics and Dynamics	3	0	0	3	3
CH-512	Organic Synthetic Methodology	3	0	0	3	3
CH-EL3	Departmental Elective-III	3	0	0	3	3
CH-513	Chemistry Lab-III	0	0	9	9	4
Total		**15**	**0**	**9**	**24**	**19**

SEMESTER-IV

Course No.	Subject	Teaching Schedule			Hours/week	Credit
		L	T	P		
CH-EL4	Departmental Elective - IV	3	0	0	3	3
CH-580	Dissertation				30	13
Total					**33**	**16**

Departmental Elective Courses

Course No.	Course Title	L	T	P	C
CH-551	Polymer and Polymer Composites	3	0	0	3
CH-552	Heterocyclic Chemistry	3	0	0	3
CH-553	Bioinorganic Chemistry	3	0	0	3
CH-554	Surface and Colloidal Chemistry	3	0	0	3
CH-555	Nanomaterials	3	0	0	3
CH-556	Advanced Physical Chemistry	3	0	0	3
CH-557	Supramolecular Chemistry	3	0	0	3
CH-558	Computational Chemistry	3	0	0	3
CH-559	Solid State Chemistry	3	0	0	3
CH-560	Biochemistry	3	0	0	3
CH-561	Advanced Polymer Technology ***(From Department of Chemical Engineering)***	3	0	0	3
CH-562	Industrial Chemical Technology ***(From Department of Chemical Engineering)***	3	0	0	3

CH-500: Inorganic Chemsitry-I
(3-0-0, 3 hours, 3 credits)

Stereochemistry and Bonding In Main Group Compounds and Metal Ligand Bonding
VSEPR, Walsh diagrams (tri and tetra-molecules), d π-p π bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules. Limitations of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, π bonding and molecular orbital theory.

Metal-Ligand Equilibria in Solution
Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by pH spectrophotometry.

Reaction Mechanism of Transition Metal Complexes-I
Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic application of valance bond and crystal field theories, kinetics of octahedral substitution.

Reaction Mechanism of Transition Metal Complexes –II
Acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, reactions without metal-ligand bond cleavage. Substitution reactions in square planar complexes, the trans effect, mechanism of substitution reaction, Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross-reactions and Marcus Hush Theory, inner sphere type reactions.

Metal Cluster
Higher boranes, carboranes, metallobranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

References:

1. Cotton, F.A.; Wilkinson *Advanced Inorganic Chemistry*, 6th edition, John Wiley& Sons, 1999.
2. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*,4th edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. *Chemistry of the Elements*, 2nd edition, Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.
4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J. Van *Magnetic Properties of Transition Metal Compounds*, Inorganic Chemistry Concepts 2, Springer-verlagNew York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. *Inorganic Chemistry*, 1st edition, Oxford University Press, 2006.
7. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.

CH-501: Organic Chemsitry-I

(3-0-0, 3 hours, 3 credits)

Nature of Bonding in Organic Molecule

Delocalized chemical bonding, conjugation, Cross conjugation, resonance hyper conjugation, Bonding in fullerenes, Tautomerism, Aromaticity in benzenoid and non benzenoid compd. Alternant and non alternant hydrocarbons, Huckel's rule. Energy level of π M.O., Annulenes, anti aromaticity, aromaticity, Homo aromaticity, PMO approach.

Bonds weaker than covalent, addition compound, crown ether complexes and cryptands, Inclusion compound, cyclo dextrins, Catenanes & rotaxanes. Effect of structure on reactivity-resonance and field effects, steric effect, quantitative treatment.

Stereochemistry

Conformational analysis of cyclo alkanes, decalins, effect of confirmation on reactivity. Confirmation of sugars, Steric strain due to undesirable crowding of resolution, entatiotropic and diasterotropic atoms. Stereo specific and stereo selective synthesis, chirality due to helical shape. Stereochemistry of compounds containing N,S,P.

Aliphatic Nucleophilic Substitution

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group mechanism, neighbouring group participation by π and σ bonds, Classical and nonclassical carbocations, norbornyl system. common carbocation rearrangements. The SN1 mechanism. Nucleophilic substitution at an allylic, aliphatic, trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile, regioselectivity.

Aliphatic Electrophilic Subsitution

Biomolecular mechanisms-SE2 and SEI. The SE1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeyer reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution

The SNAr, SN1, benzyne and SRN1 mechanisms, Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The Von Richter, Sommelet-Hauser and smiles rearrangements.

ESSENTIAL BOOKS:

1. March, Jerry *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 6th edition, John Wiley, 2007.
2. Carry, F. A.; Sundberg, R.J. *Advanced Organic Chemistry*, 3rd edition, Plenum, 1990.
3. Sykes, Peter *A Guide Book to mechanism in Organic Chemistry*, 6th edition, Longman, 1989.
4. Morrison, R. T.; Boyd, R. N. *Organic Chemistry*, 6th edition, Prentice Hall, 1992.
5. Kalsi, P. S. *Organic Reactions and their Mechanisms*, 2nd edition, New Age International Publishers, 2000.

B OOKS FOR FURTHER READING:

1. Mukherji, S.M.; Singh, S.P. *Reactions Mechanism in Chemistry*, Vol. I, II, III, Macmillan, 1985.
2. Nasipuri, D. *Stereochemistry of Organic Compounds*, 2nd edition New Age International Publishers, 1994.
3. Kalsi, P.S. *Stereochemistry of Organic Compounds*, 2nd edition, New Age International, 1993.
4. Kalsi, P.S. *Stereochemistry: Conformation and Mechanism*, 2nd edition, Wiley Eastern Limited, 1993.

CH-502: Physical Chemistry-I
(3-0-0, 3 hours, 3 credits)

Fundamentals of quantum chemistry: Basic postulates, eigenvalues and eigenvectors, Hermitian operators, applications including translational, vibrational and rotational degrees of freedom - particle in 1D/2D/3D box, particle in a ring, rigid rotor, harmonic oscillator. Electronic, vibrational and rotational transitions.Solution of SchrÖdinger equation for the hydrogen atom; radial and angular functions, atomic orbitals and electron spin. Multi-electron systems, term symbols.

Applications of Quantum chemistry: Understanding of chemical bonding: Approximate techniques: Born-Oppenheimer approximation, variation and perturbation methods with examples. Valence bond theory including mathematical treatment of sp, sp^2 and sp^3 hybridized orbitals, molecular orbital theory with suitable examples, Huckel molecular orbital approach. Introduction to semi-empirical and ab-initio methods.

Group theory: Concept of molecular symmetry and groups, symmetry operations and symmetry elements in molecules, matrix representations of symmetry operations, point groups, representation of a group, reducible and irreducible representations, great orthogonality theorem and its consequences.

Applications of group theory: Applications of group theory to atomic orbitals in ligand fields, molecular orbitals, symmetry of normal modes of vibrations, prediction of infrared, Raman active vibrational modes, and electronic transitions.

References:

1. Levine, I. N. "*Quantum Chemistry*", 7th Ed., PHI Learning Pvt. Ltd., Delhi. 2013
2. McQuarrie, D. A. "*Quantum Chemistry*" Reprint, Viva Books. 2007
3. Atkins, P. "*Molecular Quantum Mechanics*", 4th Ed., Oxford University Press. 2010
4. Cotton, F. A., "*Chemical Applications of Group Theory*", Reprint, Wiley Eastern. 1994

CH-503: Molecular Spectroscopy
(3-0-0, 3 hours, 3 credits)

Overview of molecular spectroscopy: Different aspects of molecular spectroscopy, the Born-oppenheimer approximation, transition probability, oscillator strength, the integrated absorption coefficient.

Microwave spectroscopy: Classification of the rotors, intensity of the rotational lines, population of energy levels, non-rigid rotation, anharmonicity and centrifugal distortion, effect of isotopic substitution. Rotation spectra of the linear, spherical top and asymmetric top polyatomic molecules.

Infrared and Raman spectroscopy: Types of vibration bands- overtones, combination bands, Fermi resonance phenomenon, finger print region, FTIR spectroscopy and application. Rayleigh and Raman scattering, polarizabilities, rotational and vibrational Raman spectra, selection rules, polarization of light and Raman effect, resonance Raman and coherent anti-Raman spectroscopy.

UV-visible spectroscopy: Electronic spectra, Frank-Condon Principle, predissociation spectra, Fortrat diagram, conjugated polyene and enone systems, different types of charge transfer transitions and their basis. Charge transfer spectra in organic and inorganic systems.

Photoelectron spectroscopy: The photoionization processes, Auger and autoionization processes, de-excitaion by fluorescence, outlines of UPS, XPS and Auger techniques and their applications in interpretation of valence and core shell spectra of atoms and molecules.

Magnetic resonance spectroscopy: Nuclear moments, nuclear spin states in a magnetic field and the resonance phenomenon, relaxation processes and their importance. Bloch equation, Larmor frequency, shielding constant and chemical shifts. Spin-spin coupling ,Dynamic NMR and line shapes. General introduction to double resonance experiments and nuclear overhauser effect, chemical shift reagents, multinuclear NMR. ESR Spectroscopy: Principle of ESR and interpretation of its applications for ESR spectra of $-CH_3$ and $-CH_2$ radicals.

References:

1. Banwell, C.N. and McCash, E.L.M.,"*Fundamentals of Molecular Spectroscopy*", 4th Ed. McGraw-Hill, N. Y. 1999.
2. Slichter, C.P., " *Principles of Magnetic Resonance*", Springer Verlag. 1981.
3. Graybeal, J.D., "*Molecular Spectroscopy*", McGraw-Hill. 1988.
4. Atkins, P. and Paula, J.de, "*Physical Chemistry*", 7th Ed., Oxford Univ. Press. 2003.

CH-504: Chemistry Lab-I
(0-0-9, 9 hours, 4 credits)

Inorganic Chemistry

1. Gravimetric Estimation of two constituents when present together in a given complex.
2. Analysis of two cation-system using EDTA.
3. Preparation of Tris(thiourea)cuprous(I) sulphate $[Cu(tu)_3]_2SO_4.2H_2O$ (Where tu stands for thiourea) and its physicochemical characterization including IR Study.

Organic Chemistry

1. To determine corrected melting points of an unknown organic compound (calibration of thermometer).
2. Adipic acid from cyclohexanol (oxidation).
3. p- Iodonitrobenzene from p-nitroaniline.
4. Preparation of benzyl alcohol and benzoic acid (Cannizzaro's reaction).
5. N- Bromo succinimide (Bromination).
6. Dibenzal acetone from benzaldehyde (Claisen-Schmidt reaction).
7. Cinnamic acid from benzaldehyde (Knoevenaegal reaction).
8. Acetanilide, bromoacetanilide, bromoaniline.
9. Diphenylmethane from benzylchloride (Friedel Craft's reaction).
10. Benzanilide (Schotten-Baumann reaction).
11. o-Benzoylbenzoic acid (Friedel Craft's reaction).

Physical Chemistry

1. Viscosity:
   (i) Determination of percentage composition of a liquid mixture by viscosity measurement.
   (ii) Determination of molecular weight of a polymer (say polystyrene) by viscosity measurement.
2. Surface Tension:
   (i) Determination of Parachor value for >CH2 group.
   (ii) To measure interfacial tension and to test the validity of Antonoff's rule.
   (iii) To determine the critical micelle concentration of a soap by surface tension method.
3. Colorimetry:
   (i) To verify lambert beer's law for $KMnO_4/K_2Cr_2O_7$ solutions.
   (ii) To find composition of Ferric ions-salicylic acid complex by Job's method.
   (iii) To determine the dissociation constant of phenolphthalein colorimetrically.

References:

1. Pass, G.; Sutcliffe Practical Inorganic Chemistry, 1st edition, Chapmann and Hall Ltd., 1968.
2. Jolly, W.L. Synthetic Inorganic Chemistry, 2nd edition, Prentice Hall, Inc., 1961.
3. Nakamoto, Kazuo Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5th edition, John Wiley and Sons, 1997.
4. Mendham, J; Denney, R.C.; Barnes, J.D.; Thomas, M. Vogel's Textbook of Quantitative Chemical Analysis, 6th edition, Pearson Education, Ltd., 2000.
5. 1. Harwood, L.M., Moody, C.J. Experimental Organic Chemistry, 1st edition, Blackwell Scientific Publishers, 1989.
6. Vogel, A.I. Text Book of Practical Organic Chemistry, ELBS, IVth edition, Longman Group Ltd.,1978.
7. Mann, F.G.; Saunders, B.C. Practical Organic Chemistry, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.
8. Tewari, K.S.; Vishnoi, N.K.; Mehrotra, S.N. A Textbook of Organic Chemistry, 2nd edition, Vikas Publishing House, 1976.
9. Leonard, J.; Lygo, B. Advanced Practical Organic Chemistry, Chapman and Hall, 1995.

CH-505: Inorganic Chemsitry-II
(3-0-0, 3 hours, 3 credits)

Structure, bonding and properties of transition metal complexes: Different types of ligands and coordination geometry (symmetry considerations), coordination number, isomerism (recapitulation), HSAB concept, thermodynamic stability, successive and overall stability constants, determination of stoichiometry (Job's method) and stability constants by spectrophotometric, potentiometric and polarographic methods, Irving-William series, chelate and macrocyclic effect. Stereoisomerism in inorganic complexes

Metal-ligand bonding: Overview of crystal field and ligand field theories of 4-, 5- and 6-coordinated complexes, d-orbitals splitting in linear, trigonal, octahedral, square planar, tetrahedral, square pyramidal, trigonal-bipyramidal and cubic complexes, measurement of CFSE (d_1 to d_{10}) in weak and strong ligand fields, Jahn-Teller distortion, nephelauxetic series, variation of lattice energy, ionic radii and heat of hydration across 1st row transition metal ions.

Molecular orbital theory (MOT) of coordination compounds: Composition of ligand group orbitals, molecular orbital energy diagrams of octahedral, tetrahedral, square planar complexes including both σ and π bonding, angular overlap model.

Electronic spectra of coordination compounds: Energy states from spectral terms of dn configurations, selection rules for ligand-field and charge transfer transitions in metal complexes, band intensities, factors influencing band widths, splitting of various terms, Orgel and Tanabe-Sugano diagrams of octahedral and tetrahedral dn complexes, calculation of ligand field parameters, luminescence, phosphorescent complexes.

Magnetic properties of coordination compounds: Fundamental equations in molecular magnetism, magnetic susceptibility and magnetic moment, diamagnetic and paramagnetic behavior of transition metal complexes, spin-orbit coupling effects (L-S coupling and j-j coupling), orbital angular moment and its quenching in octahedral and tetrahedral complexes, temperature independent paramagnetism (TIP) of complexes, spin cross over phenomenon, spin admixed states, metal-metal direct spin interaction and super exchange spin-spin interaction through bridging ligands, ferromagnetic, anti-ferromagnetic, ferrimagnetic behaviour of transition metal compounds, effect of temperature on their magnetic properties, single molecule magnets.

References:

1. Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons, **1999**
2. Douglas, B.E., McDaniel, D.H. and Alexander, J.J., "Concepts and Models in Inorganic Chemistry", 3rd Ed., John Wiley & Sons., **2001**
3. Figgis, B.N., and Hitchman, M.A "Ligand Field Theory and Its Applications", Wiley Eastern Ltd., **1999**
4. Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education, Inc., **2003**
5. Atkins, P., Overton, T., Rourke, J., Mark, W. and Armstrong, F., "Shriver and Atkins' Inorganic Chemistry", 4th Ed, Oxford university press. **2009**

CH-506: Organic Chemsitry-II
(3-0-0, 3 hours, 3 credits)

Reaction Mechanism, Structure and Reactivity

Types of mechanism, types of reactions, thermodynamics and kinetic requirement. Kinetic and thermodynamics control, Hammond's postulate, Curtin-Hammett Principle, The Hammett equation and linear free energy relationship, substituent and reaction constants, Taft equation.Potential energy diagrams, transition states and intermediates, method of determining mechanisms,
isotope effects.

Addition to Carbon-Carbon Multiple Bonds

Mechanistic and stereochemical aspects of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Addition to cyclopropane ring. Hydrogenation of double and triple bonds, hydrogenation of aromatic ring. Hydroboration. Michael reaction.

Addition To Carbon-Heteroatom Multiple Bonds

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds acids, esters and nitriles. Addition of grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

Free Radical Reactions

Type of free radical reactions, free radical substitution mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactivity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation. Coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free Radical Rearrangement. Hunsdiecker reaction.

Elimination Reaction

The E2, E1 and E1cB mechanisms and their spectrum, Orientation of the double bond. Reactivity effects of substrate structure, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

Pericyclic Reactions

Molecular orbital symmetry, frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reactions conrotatory and disrotatory motions 4n, 4n +2 and allyl system. Cycloadditions-antarafacial suprafacial additions, 4n and 4n+2 systems, 2+2 additiion of ketenes, 1, 3-dipolar cycloadditions and cheleotropic reactions.

Sigmatropic rearrangements-Suprafacial and antarafacial shifts of H.

Sigmatropic shifts involving carbon moieties, [3, 3]-and [5, 5]- sigmatropic rearrangements. Claisen, Cope and aza-Cope rearrangement. Fluxional tautomerism. Ene reaction. Norish type-I and II, photochemical rearrangements

Reference Books:

1. March, Jerry *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 6th edition, John Wiley, 2007.
2. Carry, F. A.; Sundberg, R.J. *Advanced Organic Chemistry*, 3rd edition, Plenum, 1990.
3. Sykes, Peter *A Guide Book to mechanism in Organic Chemistry*, 6th edition, Longman, 1989.
4. Morrison, R. T.; Boyd, R. N. *Organic Chemistry*, 6th edition, Prentice Hall, 1992.
5. Kalsi, P. S. *Organic Reactions and their Mechanisms*, 2nd edition, New Age International Publishers, 2000.

CH-507: Physical Chemsitry-II
(3-0-0, 3 hours, 3 credits)

Chemical and Ionic Equilibrium: Free energy change in a chemical reaction and its relation to reaction quotient. Thermodynamic derivation of the law of chemical equilibrium. Distinction between ΔG and ΔGo, Le Chatelier's principle. Relationshipsbetween Kp, Kc and Kx for reactions involving ideal gases.

Strong, moderate and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect. Salt hydrolysis-calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions. Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Introduction to electrochemistry: Types of electrochemical cells, Arrhenius and Debye-Huckel-Onsager theory for electrolytes, Nernst Equation, Application of EMF and conductometric measurements in determining (i) free energy, enthalpy, entropy and kinetic parameters of reactions, (ii) equilibrium constants, and (iii) solubility limits of different salts. Commonly used electrode types and their functioning. Concentration cells with and without transference, liquid junction potential; determination of activity coefficients and transference numbers. Detailed qualitative discussion of potentiometric/conductometric titrations (acid-base, redox, precipitation),

Advanced Electrochemistry: Working principle and applications of Voltammetry, Polarography and Amperometric titrations.

References:

1. Castellan, G.W., *Physical Chemistry*, Narosa, 4th Ed., 2004.
2. Barrow, G.M., *Physical Chemistry*, Tata McGraw Hill, 2007.
3. Sane, R.T. and Joshi, A.P., "*Electroanalytical Chemistry*: Theory and Applications", Quest Publications. 1999.
1. Koryta, J.; Dvorak, J.; Kavan, L. *Priniciples of Electrochemistry*, John Wiley and Sons; New York, 1993.
2. Bard, A.J. and Faulkner, L.R., "*Electrochemical Methods-Fundamentals and Applications*", John Wiley. 2000.

CH-508: Chemistry Lab-II
(0-0-9, 9 hours, 4 credits)

Inorganic

1. Preparation of Chloropentaammine cobalt(III) Chloride and its IR measurements.
2. Preparation of $[Co(en)_2Cl_2]Cl$, $Na_2[Fe(CN)_5NH_3]$. H_2O, $Cu_2(CH_3COO)_4(H_2O)_2$.
3. Preparation of $Hg[Co(CNS)_4]$ and to study its properties.
4. Preparation of cis-and trans-K $[Cr(C_2O_4)_2(H_2O)_2$ and its IR study.

Organic

1. Qualitative Analysis of mixtures of two organic solids.
2. Separation of the compounds and their identification through various steps, derivative preparation, checking the purity of components by melting point.

Physical

1. Conductometric Measurements :
   - (i) Determination of cell constant of a cell and study the effect of dilution on equivalent conductance of strong/weak electrolytes.
   - (ii) Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid like acetic acid.
   - (iii) Determination of degree of hydrolysis of a salt.
   - (iv) Conductometric titration of a weak acid with strong base.
   - (v) Conductometric titration of mixture of strong and weak acid with strong base.
   - (vi) Conductometric titration of a weak acid with weak base.
2. Potentiometry:
   - (i) Potentiometric titration of polyprotic acids with strong base.
   - (ii) Potentiometric titration of mixture of strong and weak acid with strong base.
   - (iii) Determination of pKa of weak acid/base.
   - (iv) Determination of concentration of halides in a solution.
   - (v) Determination of heat of reaction, equilibrium constant and other thermodynamic functions for following systems:
     - (a) $Zn + Cu^{2+}$ $Zn^{2+} + Cu$
     - (b) $Zn + Pb^{2+}$ $Zn^{2+} + Pb$

References:

1. Pass, G.; Sutcliffe Practical Inorganic Chemistry, 1st edition, Chapmann and Hall Ltd., 1968.
2. Jolly, W.L. Synthetic Inorganic Chemistry, 2nd edition, Prentice Hall, Inc., 1961.
3. Kolthoff, I.M.; Sanddl, E.B. Text Book of Quantitative Inorganic Analysis, Revised Edition, London Macmillan and Co. Ltd., 1950.
4. Nakamoto, Kazuo Infrared and Raman Spectra of Inorganic and Coordination Compounds: Part A and B, 5th edition, John Wiley and Sons, 1997.
5. Mendham, J; Denney, R.C.; Barnes, J.D.; Thomas, M. Vogel's Textbook of Quantitative Chemical Analysis, 6th edition, Pearson Education, Ltd., 2000.
6. Harwood, L.M., Moody, C.J. Experimental Organic Chemistry, 1st edition, Blackwell Scientific Publishers, 1989.
7. Vogel, A.I. Text Book of Practical Organic Chemistry, ELBS, IVth edition, Longman Group Ltd.,1978.
8. Mann, F.G.; Saunders, B.C. Practical Organic Chemistry, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.
9. Tewari, K.S.; Vishnoi, N.K.; Mehrotra, S.N. A Textbook of Organic Chemistry, 2nd edition, Vikas Publishing House, 1976. 5. Leonard, J.; Lygo, B. Advanced Practical Organic Chemistry, Chapman and Hall, 1995

CH-509: Organometallics
(3-0-0, 3 hours, 3 credits)

Structure and bonding in organometallics: 18 electron rule and its application to π-acceptor ligands, limitations of 18 electron rule, description of bonding models for π-acceptor ligands including CO, alkenes (Dewar-Chatt-Duncanson model) and tertiary phosphines, physical evidences and consequences of bonding.

Main group organometallics: Introduction, review of comparative aspects of synthetic methods, reactivity and bonding in ionic, covalent, electron deficient and electron rich organometallic compounds. Kinetics and mechanism of ligand substitution (associative and dissociative), oxidative addition and reductive elimination, transmetallation, migratory insertions, reactivity at metal-bound ligands.

Organotransition metal chemistry: σ-Bonded transition metal-alkyls, -aryls, -alkenyls(vinyls), -alkynyls(acetylides), reactions in σ–organyls: homolytic cleavage, reductive elimination, electrophilic cleavage, insertion, β-metal hydrogen elimination, α-abstraction or α-elimination and γ- and δ-remote C-H functionlization.

Organotransition compounds with multiple metal-carbon bonding: Transition metal-carbenes/-carbynes, -bridging carbenes/carbynes, reactions of carbene/carbine complexes such as ligand substitution, nucleophilic, electrophilic attack, dismutation, and ligand coupling reactions.

Organotransition compounds with multicenter bonds: Concept of hapticity,transition metal complexes of alkenes, Ziese salt, alkynes, allyls, butadienes; π-metal complexes of cyclobutadienes, cyclopentadienyls, arenes, cycloheptatrienyls and cyclooctatetraenes, reactions and bonding in ferrocene; stereochemical non-rigidity in organometallic compounds and fluxionalty, bimetallic and cluster complexes.

Applications of organometallics and clusters in catalysis: Alkene metathesis, Cativa and Monsanto processes for production of acetic acid, carbonylation and decarbonylation reactions, Wacker process, cyclooligomerisation of acetylene using Ni/Cr catalysts, Mobil and Fischer-Tropsch processes, polymer-bound catalysts, metal carbonyl clusters in catalysis.

References:

1. Huheey, J.E., Keiter, E.A. and Keiter, R.L., "Inorganic Chemistry Principle of Structure and Reactivity", 4th Ed, Pearson Education Inc., **2003**
2. Cotton, F.A., Wilkinson, G., Murillo, C.A. and Bochmann, M., "Advanced Inorganic Chemistry", 6th Ed., John Wiley & Sons, **1999**
3. Hill, A.F., "Organotransition Chemistry", The Royal Society of Chemistry, Cambridge., **2002**
4. Bochmann, M. (Ed.), "Oxford Premier Series on Organometallics", Vol. 1 and 2, Oxford Press., **2002**
5. Gupta, B.D. and Elias A.J., "Basic Organometallic Chemistry", 2nd Ed., University Press (India) Pvt. Ltd., **2013**

CH-510: Interpretative Molecular Spectroscopy
(3-0-0, 3 hours, 3 credits)

Electronic spectroscopy: Electronic transitions in organic molecules, Woodward-Fieser rules for alkenes, Woodward rules for enones, aromatic compounds.

Infrared and Raman spectroscopy: For simple organic molecules, predicting number of active modes of vibrations, analysis of representative spectra of compounds with various functional groups, application of isotopic substitution.

Mass spectrometry: Basic principles, hard and soft ionization techniques, mass analyzer in ESI-MS and MALDI-MS, high resolution MS, isotope abundance, molecular ion, fragmentation processes (McL) of organic molecules, deduction of structure through mass spectral fragmentation.

Nuclear magnetic resonance: Effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant *J*, first order and second order spectra, examples of AB, AX, ABX, AMX and AA′BB′ systems, simplification of second order spectrum, selective decoupling, double resonance, use of chemical shift reagents for stereochemical assignments, 13C NMR, T1 relaxation, NOE effects, DEPT, determination of number of attached hydrogens,1H and 13C chemical shifts to structure correlations, study of dynamic processes by VT NMR, restricted rotation (DMF, DMA, biphenyls, annulenes), cyclohexane ring inversion, degenerate rearrangements (fullvalene and related systems). Multinuclear NMR, COSY, DQF-COSY, HETCOR, HMQC, HMBC, TOCSY, ROESY, VGSE.

Combined Spectroscopic applications: Structure elucidation of organic/inorganic compounds using spectroscopic methods.

References:

1. Silverstein, R. M., Webseter, F. X. and Kiemle, D., "Spectrometric Identification of Organic Compounds", 7th Ed., John Wiley & Sons. **2005**
2. Kemp, W. L., "Organic Spectroscopy", Palgrave. **2008**
3. Pavia, D. L., "Spectroscopy", 4th Ed., Cengage. **2012**
4. Williams, D. and Fleming, I., "Spectroscopic Methods in Organic Chemistry", 6th Ed., McGraw Hill Education (India) Private Limited., **2011**

CH-511: Molecular Energetics and Dynamics
(3-0-0, 3 hours, 3 credits)

Statistical Thermodynamics: Statistical view of entropy. Laws of thermodynamics from statistical considerations. Molecular view of temperature and heat capacity. Boltzmann distribution.
Thermodynamic quantities in terms of partition functions. Statistical mechanics of simple gases and solids. Kinetic theory of gases. Equilibrium constant, mean energies and heat capacities in terms of partition functions. Bose-Einstein and Fermi-Dirac statistics. Use of Statistical Thermodynamics in understanding molecular interaction in liquids.

Chemical Kinetics: Differential and integrated rate laws for zero, first and second order reactions. Complex Reactions. Catalysis. Temperature dependence and Arrhenius law.
Potential energy surfaces. Kinetic theory of collisions. Transition state theory. RRK and RRKM theories. Reaction cross-sections, rate coefficients, reaction probabilities. Enzyme catalysis and homogeneous catalysis. Salt effects. Photochemical reactions. Ultrafast reactions.

References:

1). Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology/ by K. A. Dill and S. Bromberg, Garland Science, 2003.
2). Molecular Thermodynamics by D. A. McQuarrie, and J. D. Simon, Viva Books, 2004.
3). Atkins' Physical Chemistry by P. Atkins and J. De Paula, 8th edition, Oxford University Press, 2006.
4). Chemical Kinetics by K. J. Laidler, 3rd Edition, Prentice Hall, 1987.
5). Chemical Kinetics and Dynamics by J. I. Steinfeld, J. S. Francisco and W.L. Hase, 2nd Edition, Prentice Hall, 1999.
6). Chemical Kinetics and Reaction Dynamics by P. L. Houston McGraw-Hill Higher Education, 2001.

CH-512: Organic Synthetic Methodology
(3-0-0, 3 hours, 3 credits)

Oxidations: Oxidations of hydrocarbons (alkanes, alkenes and aromatic), alkenes to epoxides (peroxides/per acids based), Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation, alkenes to diols (Manganese, Osmium based), Sharpless asymmetric dihydroxylation, Prevost reaction and Woodward modification, alkenes to carbonyls with bond cleavage (manganese, osmium, ruthenium and lead based-ozonolysis), alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, selenium, chromium based allylic oxidation), ketones to α-hydroxy ketones, α,β-unsaturated ketones, ester/lactones (Baeyer-Villiger), alcohols to carbonyls (chromium, manganese, aluminum, silver, ruthenium, DMSO, hypervalent iodine and TEMPO based reagents), alcohols to acids or esters, phenols (Fremy's salt, silver carbonate).

Name reactions: Baylis-Hillman reaction, Henry reaction, Nef reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Tishchenko reaction, Ugi reaction, Brook rearrangement and Tebbe olefination.

Protection and deprotection of functional groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds, chemo- and regioselective protection and deprotection, illustration of protection and deprotection in multi-step synthesis.

Retrosynthetic analysis: Basic principles and terminology of retrosynthesis, guidelines, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions, reversal of polarity (umpolung).

References:

1. Carey, F. A. and Sundberg, R. J., "Advanced Organic Chemistry, Part B: Reactions and Synthesis", 5th Ed., Springer, 2007
2. Carruthers, W. and Coldham, I., "Modern Methods of Organic Synthesis", 4th Ed., Oxford University Press, 2004
3. Smith, M.B., "Organic Synthesis", 3rd Ed., Academic Press. 2010

CH-513: Chemistry Lab-III
(0-0-9, 9 hours, 4 credits)

Inorganic

1. Colorimetric estimation of cations and anions.
2. Separation techniques
   (i) Ion exchange (ii) Solvent extraction (iii) Column and paper chromatography

Organic

1. Preparation of the following organic compounds:
   1. Hydroxynaphthaldehyde (Reimer tiemann Reaction)
   2. Benzoin. Benzil. Benzilic acid.
   3. Benzophenone, Benzophenone oxime, Benzanilide (Beckmann Rearrangement).
   4. Trinitrophenol (picric acid) and picrate derivative.
2. Studies of TLC, column chromatography and paper chromatography for organic mixture.

Physical

1. Polarimetry:
   (i) Determination of the specific and molecular rotation of sucrose at different concentrations and to obtain the value of intrinsic rotation for sucrose.
   (ii) To study the kinetics of inversion of cane sugar by optical rotation measurement.

2 . Chemical Kinetics :
   (i) To compare the strengths of two acids by studying hydrolysis of an ester.
   (ii) To study the kinetics of hydrolysis of ethyl acetate by NaOH.
   (iii) Determine the specific reaction rate of the potassium persulphate-iodide reaction by initial rate method.
   (iv) To study the kinetics of iodination of acetone in the presence of acid by initial rate method.
   (v) To study the kinetics of saponification of ethyl acetate by NaOH conductometrically.
   (vi) To study the iodination of acetone using a colorimeter.

References:

1. Harwood, L.M., Moody, C.J. Experimental Organic Chemistry, 1st edition, Blackwell Scientific Publishers, 1989.
2. Vogel, A.I. Text Book of Practical Organic Chemistry, ELBS, 5th edition, Longman Group Ltd.,1989.
3. Mann, F.G.; Saunders, B.C. Practical Organic Chemistry, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1981.
4. Tewari, K.S.; Vishnoi, N.K.; Mehrotra, S.N. A Textbook of Organic Chemistry, 2nd edition, Vikas Publishing House, 1976.
5. Leonard, J.; Lygo, B. Advanced Practical Organic Chemistry, Chapman and Hall, 1995. Pass, G.; Sutcliffe Practical Inorganic Chemistry, 1st edition, Chapmann and Hall Ltd., 1968.
6. Jolly, W.L. Synthetic Inorganic Chemistry, 2nd edition, Prentice Hall, Inc., 1961.
7. Mauritis Kolthoff's and Sanddle Text Book of Quantitative Inorganic Analysis.
8. Vogel, A.I. Text Book of Practical Organic Chemistry, ELBS, 5th edition, Longman Group Ltd.,1989.

Departmental Electives

CH-551: Polymer and Polymer Composites
(3-0-0, 3 hours, 3 credits)

Basic concepts (classification, nomenclature, molecular weight and distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationship), Methods of determination of molecular weight, distribution, size and shape of macromolecules, Mark-Houwink relationship, Thermodynamics of polymer solutions, Rubber elasticity concepts, thermodynamic equation of state, theories

Polymerization Techniques - bulk, solution, emulsion- description of the process, progress of polymerization, rate of polymerization, degree of polymerization, suspension, living radical polymerization technique. Mechanical properties of polymers and methods of determination, ielected commercial polymers and applications

Introduction to composite materials, comparison of different materials with composites - advantages and disadvantages, Principles of composite reinforcement, Effect of fibrous reinforcement on composite strength, Types of reinforcement such as natural, glasses, carbon/graphite, aramid fibers, high strength and high modulus fibers, Surface treatment and various forms of fibers.
Processing and production techniques like hand-layup, bag moulding, filament winding, pultrusion, Prepegs, their manufacture and characterization, Sheet moulding and dough moulding compounds and their processing, resin transfer mouldings.

Role of polymers for high-tech areas such as light emitting diode, OSR in satellite communication, photovoltaic etc, High temperature polymers such as polyimides, polyetherimides, PEEK, silicone etc, their preparations, properties & applications, Liquid Crystalline, polymers - their synthesis and properties of such polymers and applications, self reinforced composites, Concept of nanofillers and polymer nanocomposites. High energy absorbing polymer, Super absorbent polymers - their synthesis, properties and applications' Polymers, for biomedical applications.

References:

1. Introduction to Physical Polymer Science, L. H. Sperling, Wiley Interscience, New York, 1986.
. Principles of Polymerization, G. Odian, Third edition, Wiley Interscience. New York, 1992.
3. Principles of Polymer Chemistry, P. J. Flory, Cornell University Press, Ithaca, 1953.
4. Textbook of Polymer Science, F. W. Billmeyer, 3rd Edition, John Wiley, London, 1994.
5. "Polymer Science", Gowariker et al, Wiley Eastern, New Delhi, 1990.
6. Hand Book of Composites, by George Lubin.
7. Hand Book of Fibre glass and Advanced Plastic Composites, by G. Lubin
8. Reinforced Palstic Handbook by Rosato & Rosato.
9. Polymer Science and Technology, by J. R. Fried.
10. Nanocomposite Science and Technology by Pulickel M. Ajayan, Linda S. Schadler, Paul V. Braun Hardcover, September 2003 Wiley

CH-552: Heterocyclic Chemistry

(3-0-0, 3 hours, 3 credits)

Heterocycles: Systematic nomenclature of heterocyclic compounds (Hantzsch-Widman, replacement and fusion methods), biological importance of heterocyclic compounds.

Five-membered heterocycles with one heteroatom: Chemical structures of furan, pyrrole and thiophene, and degree of aromaticity. General syntheses methods for 5-member rings. Paal-Knorr, Feist-Benary, Hantzsch and Knorr syntheses. Electrophilic substitution, reactants employed and orientation of the substituent on the ring.

Benzo derivatives of five-membered heterocycles with one heteroatom:
Preparation of indole and carbazole derivatives. Fisher, Bischler, Madelung and Reissert syntheses. Preparation and reactivity of benzofurans (coumarins), benzothiophenes, dibenzofurans and dibenzothiophenes.

Pyridines, quinolines and isoquinoles: Influence of the imine group on the reactivity of the pyridine ring. Nucleophilic and electrophilic substitutions on pyridine, quinolines and isoquinolines. Comparison of reactivity with benzene and naphthalene. Preparation of pyridine salts and pyridine *N*-oxides and synthetic applications. Skraup, Friedlander, Pfintzinger Bischler-Napieralski and Pictet syntheses.

Heterocycles with 5 or 6 members and two or three heteroatoms: Syntheses and reactivity of oxazoles, thiazoles, oxadiazoles, thiadiazoles, benzothiazoles, benzothiadiazoles, triazole, benzotriazole, pyrimidines, pyrazines, quinoxalines and triazines

New materials derived from heterocycles: Syntheses of indigo, mauveine, cyanines, tetrathiafulvalenes and related dyes, organic sensitizers for DSSC, electron donors and acceptors for organic solar cells, optical chemosensors and organic semiconductors for thin-film transistors.

References:

1. Gilchrist, T. L., "Heterocyclic Chemistry", 3rd Ed., Pearson Education, India. (ISBN: 978-0582278431)., 2007
2. Joule, J. A. and Mills, K., "Heterocyclic Chemistry", Wiley-Blackwell. (ISBN: 978-1-4051-3300-5), **2010**
3. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin, V. V., "Handbook of Heterocyclic Chemistry", 3rd Ed., Elsevier. (ISBN: 978-0-08-095843-9), 2010
4. Gupta, R. R., Kumar, M. and Gupta, V., "Heterocyclic Chemistry, Vol. I: Principles, Three- and Four-Membered Heterocycles", Springer. (ISBN: 978-3-642-72278-3), 1998
5. Gupta, R. R., Kumar, M. and Gupta, V., "Heterocyclic chemistry, Vol. II: Five-Membered Heterocycles", Springer. (ISBN: 978-3-642-08460-7), **1998**
6. Sainsbury, M., "Heterocyclic Chemistry", Wiley. (ISBN: 978-0-471-28164-1) 2002

CH-553: Bioinorganic Chemistry

(3-0-0, 3 hours, 3 credits)

Inorganic biochemistry: Metalloproteins and enzymes– Role of metal ions in the active sites, structure and functions of metalloproteins and enzymes containing Mg, Ca, V, Mn, Fe, Co, Ni, Cu and Zn ions. Detailed structure and mechanistic studies of the following–Mn-photosystem-II, catalase, pseudocatalase, oxygen carriers, haemoglobin, myoglobin, non-porphyrin oxygen carriers, hemerythrin, hemocyanin, Fe-ribonucleotide reductase, cytochrome c oxidases, cytochrome P-450s, Ni-urease, hydrogenase, nitrogen fixation, Cu-blue copper protein, tyrosinase, galactose oxidase, superoxide dismutases, Zn-carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, Mo and W containing enzymes, xanthine oxidase.
Biological importance of Vitamin B12 and coenzymes, and their biomimetic studies.

Chemical toxicity and metallotherapy: Toxic chemicals in the environment, toxic effects of arsenic, cadmium, lead, mercury, carbon monoxide, cyanide and other carcinogens, metal containing drugs in therapy, interaction of heavy metal ions with DNA, DNA cleavage, structure-activity relationship and mode of action. Organometallic compounds as therapeutic drugs and enzyme inhibitors.

Metal ions and diseases: Role in Alzheimer's disease– Aggregation of proteins, role of copper, zinc and iron.

References:

1. Mukherjee, G.N. and Das, A., "Elements of Bioinorganic Chemistry", Ist Ed., U.N. Dhur & Sons Pvt. Ltd., Calcutta.
2. Bertini, I., Gray, H.B. Lippard, S.J. and Valentine, J.S. "Bioinorganic Chemistry", University Science Book, South Asian Edition Reprint., **2004**
3. Lippard, S.J. and Berg, J., "Principles of Bioinorganic Chemistry", University Science Books, U.S.A., **1994**

CH-554: Surface and Colloidal Chemistry

(3-0-0, 3 hours, 3 credits)

Surfactants and Interface chemistry: Classification, micellization, c.m.c. and its determination. Shape and structure of micelles, effect of additives on micellization, thermodynamics of micellization, solubilization and applications, effect of electrolytes on solubilization. Macro and micro emulsions, dispersion and aggregation of solids by surfactants.

Membranes and their Applications: Artificial and natural membranes, Donnan membrane equilibrium, transport of electrolytes, membrane potential and ion selective electrodes.

Adsorption on solids and porous materials: Model for multilayer adsorption, BET isotherm and application to different types of adsorbents, adsorption by porous, non-porous and microporous solids. Estimation of specific surface area and pore size distribution. Special problems encountered with very narrow pore size material and adsorption from liquid phase.

Colloid systems and their properties: Origin of the charges, electro-kinetic phenomena, electrophoresis, electroosmosis, sedimentation and streaming potential. The concept of electrical double layer and various models to explain its structure and properties, DLVO theory and stability of colloids.Smoluchowski theory of kinetics of coagulation and distribution of colloids aggregates. Organic and inorganic gels and clay colloids.

Methods to detect interfacial phenomena: Principle and instrumentation of ATR-FTIR spectroscopy, SFG spectroscopy.

References:

1. Hunter, R. J., "*Foundation of Colloid Science*", Oxford Univ. Press. 2009
2. Lyklema, J., "*Fundamentals of Interface and Colloid Science*", Academic Press San Diego. 2000
3. Adamson, A.W.,"*Physical Chemistry of Surfaces*", 5th Ed., John Wiley and Sons, New York. 1990
4. Kruyt, H.R., "*Colloid Chemistry*" Vol. I & II. Elsevier Press. 1991
5. Greg, S.J. and Singh, K.S.W., "*Adsorption, Surface Area and Porosity*", 2nd Ed., Academic Press., U. K. 1982.

CH-555: Nanomaterials
(3-0-0, 3 hours, 3 credits)

Introduction to nanoscale materials: The nano-length scale, quantum confinement effect, consequences of quantum confinement of electrons, conceptual development of band theory – from molecules to clusters/quantum dots to macroscopic crystals, material dependence of nanoscale and quantum size-effect, consequences of carrier confinement in semiconductors and metals.

Structure of nanomaterials: Crystalline and amorphous nanomaterials, nanocrystals, surface energy and crystal facets, equilibrium shape of nanocrystals, surface energy as a function of surface curvature, chemical potential and solubility as a function of surface curvature and particle size, Ostwald ripening, nucleation and growth of nanoparticles.

Synthesis and applications of nanomaterials: Concepts of top-down and bottom-up approaches, chemical, aerogel, aerosol, spray-pyrolysis, microemulsion, solvothermal, sonochemical, and microwave methods of synthesis. Reactivity studies by adsorption–SO_2, CO_2, H_2S, CCl_4 and chemical warfare agents, destructive adsorption, detoxification by adsorption, air purification, desulphurization, biocidal applications, modification of nanocrystalline metal oxides and their applications.

Characterisation of nanomaterials: Surface area measurement, determination of size and texture, composition and elemental analysis.Electron probe methods (Scanning Electron Microscopy, Transmission Electron Microscopy); Scanning probe microscopy methods (Atomic Force Microscopy and Scanning Tunneling Microscopy.

References:

1. Klabunde, K.J. (Ed.), "*Nanoscale Materials in Chemistry*", WileyInterscience, New York. 2001.
2. Schmid, G. (Ed.), "*Nanoparticles: From Theory to Application*", WileyVCH, Weinheim. 2004.
3. Cao, G. and Wang, Y., "*Nanostructures and Nanomaterials*: Synthesis, Properties and Applications", 2nd Revised Ed., World Scientific. 2011.
4. Rao, C.N.R., Müller, A. and Cheetham, A.K., "*The Chemistry of Nanomaterials: Synthesis, Properties and Applications*", Vol. 1 and 2, Wiley-VCH Verlag, Weinheim. 2004.

CH-556: Advanced Physical Chemistry
(3-0-0, 3 hours, 3 credits)

Advanced chemical kinetics: Kinetics of simple and complex reactions, theories of unimolecular reactions, kinetics-proton transfer and electron transfer reactions, fast reactions–rapid flow, stopped-flow and relaxation techniques, molecular beam method, diffusion controlled reactions, oscillatory reactions, linear free energy relationship, elucidation of mechanism from kinetic data.

Irreversible Thermodynamics: Meaning and scope of Irreversible Thermodynamics, thermodynamic criteria for non-equilibrium states, phenomenological laws – linear laws, Gibbs equation, Onsager's reciprocal relations, entropy production, Prigogine's principle of maximum entropy production, non-equilibrium stationary states.

Advanced quantum chemistry: Dirac Bra-ket notation, addition of angular momentum, use of ladder operators– rigid rotor and harmonic oscillator, variation method– treatment of He atom, perturbation method– examples of anharmonic oscillator, He atom, Stark and Zeeman splitting, Hartree-Fock method.

References:

1. Laidler, K.J., "*Reaction Kinetics*", Anand Sons, New Delhi. 2005.
2. Katchalsky, A &Curren, P. F. "*Non-Equilibrium Thermodynamics in Biophysics*", Harvard University press. 1965.
3. McQuarrie, D. A. "*Quantum Chemistry*" Reprint, Viva Books. 2007
4. Atkins, P. "*Molecular Quantum Mechanics*", 4th Ed., Oxford University Press. 2010

CH-557: Supramolecular Chemistry

(3-0-0, 3 hours, 3 credits)

Fundamentals of supramolecular chemistry: Definitions, brief overview and examples; types of non-covalent interactions (H-bonding, electrostatic (ion-ion, ion-dipole, dipole-dipole), hydrophobic and steric, π-π, van der Waals), concepts of hostguest complexation with examples from ionophore chemistry, complexation of ions, molecular baskets, chalices and cages– podands, crown ethers, cryptands, calixarenes, macrocyclic effect, complexation of neutral molecules, self-assembly, molecular boxes and capsules, self-complementary species and self-replication.

Supramolecular chemistry and biological processes: Cation binding (biological relevance, affinity and selectivity, artificial ionophores, natural and artificial cation channels). Anion and neutral molecule binding –relevance factors affecting affinity and selectivity, anion and neutral molecule binding in biology, artificial hosts for anions, katapinands, guanidinium receptors, receptors based upon Lewis acid-base concepts, enantio-selective anion recognition, cyclodextrins, anion binding based upon ion-dipole interactions, simultaneous anion-cation binding, neutral molecule recognition and binding.

Synthesis of supramolecules: Synthesis of macrocycles, synthesis of receptors for cations anions, and neutral molecules, non-covalent synthesis, metal directed selfassembly of complex supramolecular architecture– rotaxanes, catenanes.

Physical methods in supramolecular chemistry: Spectroscopy in supramolecular chemistry, determination of stoichiometry, stability constants, and geometry of complexes, binding constant determination, dynamics of supramolecular systems (solid state *vs* solution behavior).

Application of supramolecular chemistry: Supramolecules in catalysis, as membrane transport, sensors, phase-transfer catalysts, supramolecular devices and switches, memories, logic gates and related systems, molecular scale machines (mechanical rotors, gears and brakes), conversion of light into fuels and light into electricity.

References:

1. Steed, J.W. and Aswood, J.L., "Supramolecular Chemistry", Wiley. **2000**
2. Dodziuk,,H., "Introduction to Supramolecular Chemistry", Springer, ISBN 1402002149., **2001**
3. Beer, P.D., Gale, P.A. and Smith, D.K., "Supramolecular Chemistry", Oxford Chemistry Printers, ISBN-10: 0-19-850447-0., **1999**
4. Cragg, P., "A Practical Guide to Supramolecular Chemistry", Wiley-VCH, ISBN: 0-470-86654-3., **2005**
5. Schneider, H.J. and Yatsimirsky, A., "Principles and Methods in Supramolecular Chemistry", Wiley-VCH, ISBN: 0-471-97253-3.

(66)

CH-558: Computational Chemistry
(3-0-0, 3 hours, 3 credits)

Fundamentals of electronic structure: Basis function–hydrogen-like, Slatertype and Gaussian type orbitals, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization and diffuse basis sets, correlation consistent basis sets, basis set super position error, energy minimization methods–derivative and non-derivative methods-simplex method, steepest descents method, Newton-Raphson method, minima, maxima and saddle points.

Semi empirical and Abintio methods: Approximation methods, self-consistent field treatment of polyatomic molecules, closed shell systems–restricted HartreeFock calculations, open shell systems–ROHF and UHF calculations, The Roothan–Hall equations, Koopman's theorem, HF limit and electron correlation, introduction to post Hartree-Fock and density functional methods.

Electronic properties: Dipole moment, electrostatic potential, frequencies, population analysis, Mulliken and Lowdin analysis, solvent effects, polarizable and nonpolarizable models.

Introduction to simulation methods: Molecular mechanics, Monte carlo and molecular dynamics simulations, periodic boundary conditions, radial distribution function, calculation of thermodynamic properties.

References:

1. Jensen, F., "*Introduction to Computational Chemistry*", John Wiley & Sons Ltd. 1999
2. Leach, A., "*Molecular Modeling: Principles and Applications*", Prentice Hall. 2001
3. Cramer, C. J., "*Essentials of computational chemistry: Theories and models*", John Wiley & Sons. 2002.
4. Levine, I. N. "*Quantum Chemistry*", 7th Ed., PHI Learning Pvt. Ltd., Delhi. 2013

CH-559: Solid State Chemistry

(3-0-0, 3 hours, 3 credits)

Symmetry in the crystalline state: Crystal symmetry, elements of translation - screw axis and gl planes, symmetry in a cube, crystal classes, stereographic projection of crystal systems, spa symmetry and space groups, HermannMauguin and Schoenflies notations, Wyckoff positio representation of monoclinic and orthorhombic space groups.

X-Ray diffraction: Crystal planes and directions, Bragg's law in reciprocal space and Ewald sphe structure factor, integrated intensity and systematic absences/presences, indexing and simulation powder X-ray diffraction patterns for simple systems.

Crystal chemistry: Hard sphere model, structures derived from HCP and CCP packing, cryst structures of various compositions, derived structures and polytypes, non-stoichiometry in solid atomic order/disorder in solids, single crystals, polycrystals, quasicrystals, amorphous / glassy solids.

Bonding in solids: Bonding in molecular solids – polymorphism, bonding in extended solids - ionic covalent and metallic. Band theory of solids - classification of semiconductors, metals and insulators free electron theory, Bloch's theorem, concept of density of state and elementary band theory, band structures of one-, two- and three- dimensional solids, selected metals and insulators.

Properties of solids: Thermal, electrical, magnetic and dielectric properties of solids.

References:

1. West, A. R., "*Solid State Chemistry and its Applications*", Reprint, Wiley India. 2013.
2. Rao, C.N.R. and Gopalakrishnan, J., "*New Directions in Solid State Chemistry*", 2nd Ed., Cambridge University Press. 1997.
3. Stout, G.H. and Jensen, L.H., "*X-Ray Structure Determination: A Practical Guide*", 2nd Ed., Wiley-Interscience. 1989.
4. Giacovazzo, C., Artioli, G. and Monaco, H. L., "*Fundamentals of Crystallography*", Oxford University Press. 2006.
5. S. Nicola, "*Magnetic Materials: Fundamentals and Device Applications*", Cambridge University, Press. 2003.

CH-560: Biochemistry

(3-0-0, 3 hours, 3 credits)

Introduction to Chemical Biology

Chemical principles of biological systems; structure of amino acids, proteins and nucleic acids; Primary, secondary, tertiary structures of proteins, Motifs of protein structure, Folding and flexibility of protein structures, protein folding thermodynamics, carbohydrate and fatty acid metabolism; basic knowledge on DNA replication and transcription; RNA processing and translation.

Techniques for Bioseparation

Method of solubilization, Chromatographic separation techniques: gel-filtration, ion exchange, affinity

Enzymes

Enzyme kinetics, enzyme catalysis, enzyme activators, enzyme inhibitors and inhibition mechanisms

Spectroscopic Tools in Biology

Different spectroscopic methods like absorption, fluorescence, surface plasmon resonance; circular dichroism, infrared, NMR and different mass spectrometric techniques

References:

1. Biochemistry, Fourth Edition, by Donald Voet and Judith G. Voet.
2. Biochemistry by Jeremy M. Berg, Lubert Stryer, John L. Tymoczko, 2002
3. Lehninger Principles of Biochemistry by David L. Nelson, 2012
4. Introduction to Protein Structure, Second Edition, by Carl Branden and John Tooze

CH-561: Advanced Polymer Technology

(3-0-0, 3 hours, 3 credits)

Introduction: Molecular weight distribution, glass transition, morphology, viscosity vs. molecular weight and mechanical property vs. molecular weight relationships, Methods of determination of molecular weight, distribution, size and shape of macromolecules, Mark-Houwink relationship, Thermodynamics of polymer solutions, Rubber elasticity concepts, thermodynamic equation of state.

Polymerization Techniques- bulk, solution, emulsion-description of the process, progress of polymerization, rate of polymerization, degree of polymerization, suspension, living radical polymerization technique, Mechanical properties of polymers and methods of determination, selected commercial polymers and applications.

Polymer modifications and recent technological advances toward live cell encapsulation and delivery, Surface modification of natural fibers for reinforcement in polymeric composites, Biopolymers based stimuli-sensitive functionalized graft copolymers as controlled drug delivery systems.

Speciality Polymers: Role of polymers for high-tech areas such as light emitting diode, OSR in satellite communication, photovoltaic etc., High temperature polymers such as polyimides, polyetherimides, PEEK, silicone etc., their preparations, properties & applications, Liquid Crystalline polymers- their synthesis, properties and applications, High energy absorbing polymer, Super absorbent polymers - their synthesis, properties and applications.

Books and References:

1. Surface modification of Biopolymers, V. K. Thakur and A.S. Singha (Ed.), John Wiley & Sons, 2015.

2. Introduction to Physical Polymer Science, L.H. Sperling, Wiley Interscience, New York, 1986.

3. Principles of Polymerization, G. Odian, Third edition, Wiley Interscience. New York, 1992.

4. Principles of Polymer Chemistry, P.J. Flory, Cornell University, Press Ithaca, 1953.

5. Textbook of polymer Science, F.W. Billmeyer, 3rd Edition, John Wiley, London, 1994.

6. Polymer Science, Gowariker et al, Wiley Eastern, New Delhi, 1990.

7. Polymer Science and Technology by J. R. Fried.

CH-562 Industrial Chemical Technology
(3-0-0, 3 hours, 3 credits)

Dyes: Structure and properties, Natural colours/dyes for textile applications, Natural food colours and their health aspects, Biomedical applications of dyes: Photodynamic therapy, Dyes in 8 bioanalysis and medical diagnostics, DNA sequencing, Cancer detection, activity with diazonium salts, Dyes as therapeutic agents.

Sugar Technology: Introduction to sugar industry, Specification of raw sugar, Refining quality of raw sugar – evaluation, calculation of raw value, By-products and co-products of sugar industry

Chemistry of Food Preservatives: Objectives and techniques of food preservation; Structure, properties and use of foods preservative: chemical preservative, biopreservative including antibiotics.

Petrochemicals – Structure, Properties and Applications: Types of crude oil, Properties of Petroleum oil products: Definition and significance of various properties like API gravity, Aniline point, Diesel index, Cloud point, Pour point, Flash point, Fire point, Smoke point, Octane number, Cetane number, Softening point; Manufacturing process of Chemicals from methane: synthesis of methanol, Acetic acid, Vinyl Acetate, Poly Vinyl Acetate, Specific requirements for automotive lubricants, oxidation deterioration and degradation of lubricants, additives and additive mechanism, synthetic lubricants.

Books and References:

1. Functional Dyes, S H Kim, Elsevier BV 2006
2. Industrial Dyes-Chemistry, Properties, Applications by Klaus Hunger WILEY-VCH Verlag, 2003
3. Natural Dyes and their Applications in Textiles by M. L. Gulrajani, IIT Delhi
4. Natural Food Colorants by Gabriel J. Lauro and F. Jack Francis (eds), Marcel Dekker Inc.
5. Manufacture and Refining of Raw Cane Sugar – V E Baikow
6. Industrial Utilisation of Sugarcane & Its Co-products - P J Manohar Rao
7. Technology of Food Preservation by Desrosier
8. Modern Petroleum Refining Processes, B. K. Bhaskara Rao
9. Lubrication – A practical guide to lubricant selection by A.R.Lansdown — Pergamon press – 1982.